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MASSACHUSETTS INSTITUTE OF TECHNOLOGY

LINCOLN LABORATORY

RESONANCE SCATTERING OF LYMAN-α RADIATION BY HYDROGEN IN THE GROUND STATE

H. E. MOSES

Group 35

TECHNICAL NOTE 1966-14

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ABSTRACT

We consider the problem of the scattering of a photon by hydrogen in the ground state when the photon has its principal frequencies near that of Lyman-α radiation. We obtain the scattering operator and cross-section for this process.

Our procedure is to adapt Dirac's theory of resonance scattering to the problem and, by quantizing the electromagnetic field in an angular momentum basis, to solve the problem exactly within the framework of the Dirac theory.

We find that the total scattering cross-section at resonance is 7.062×10^{-12} cm.^{2}. The natural half width of the scattered line is 1.03×10^{-4} A. The resonance frequency itself is shifted toward the long wave length side by 4281 mc/sec.

The shift in the resonance from the original Lyman-α frequency can be interpreted as an indication that the Dirac resonance scattering theory contains a large part of the Lamb shift of the ground state. This fact suggests new ways of obtaining the Lamb shift for various levels which will be explored in later papers.

Accepted for the Air Force
Franklin C. Hudson
Chief, Lincoln Laboratory Office

I. INTRODUCTION AND SUMMARY

It is remarkable that, despite the existence of a large body of literature on the theory of resonance scattering and on its application to problems in nuclear and atomic physics where the particle which is being scattered has non-zero mass, there have been no numerical calculations for the resonance scattering of photons by atoms or nuclei. While it is true that there are some formulas for this problem (see e.g. reference 1), these formulas seem not to have been used to obtain numerical results. The existing formulas for the resonance scattering of light as given, for example in reference 1, are obtained in such an unsystematic manner that one is discouraged from using them for fear that the result will not be very meaningful. It is perhaps for this reason that no numerical calculations exist.

To correct this deficiency of a quantum theory for the resonance scattering of light by an atom or nucleus we have undertaken a series of investigations which culminate in the calculation of the resonance scattering cross section for hydrogen atoms in the ground state when the frequency of the light is near or at that which is necessary to raise the atom to its first excited state. We have concentrated our attention on hydrogen because the wave functions are simple enough to permit evaluation of the various integrals which occur. Of course, this case is of great interest in its own right, for obvious astrophysical applications. However, the techniques which we have developed can be used when the scatterer is any atom or nucleus, provided the wave functions are known.

For our treatment we have considered only the simplest model for the hydrogen atom, namely that of a spinless electron bound to the nucleus by a Coulomb potential. The extension to the relativistic Dirac electrons appears to offer no difficulty other than the necessity of evaluating more complicated integrals and we hope to treat this case later.

In the Dirac approximation one sets some of the matrix elements of the interaction equal to zero, retaining only those which are large in the resonance region. If one regards the interaction as consisting only of this Dirac interaction, the resulting quantum mechanical problem can be solved exactly. That is, in the Dirac resonance theory one replaces the exact problem by an approximate one which can be solved exactly. Thus it is unnecessary and even incorrect to ignore retardation effects (i.e. setting $\exp i\underset{\sim}{k}\cdot\underset{\sim}{x} \simeq 1$ in matrix elements) as one frequently does in the semi-classical and quantum theory of emission and absorption of photons. Use of the exact Dirac resonance theory gives us more accurate values for the scattering line breadth and shift in the position of resonance than could be obtained by ignoring retardation.

The fact that the Dirac approximation can be solved exactly does not seem to have been widely appreciated until the appearance of reference 3, where the Dirac approximation is treated as a rigorous problem in spectral theory for certain rather general situations. Our approach to the problem is strongly influenced by reference 3.

The present paper is intended to provide a summary of results and only a sketch of the procedure used to obtain them. A more

detailed derivation will appear later in a series of papers which are still to be written.

Finally, in this present section we shall give some results:

Let us consider a light wave (photon) of frequency ν moving along the positive z-axis toward a hydrogen atom in the ground state.

We shall assume that the light wave has a specific circular polarization. Then the differential cross section for scattering in the solid angle $d\Omega$ is

$$dA = 0.8431 \times 10^{-11} \text{ cm.}^2 \cos^4 \frac{\theta}{2} C(\nu) d\Omega \qquad (1.1)$$

for scattered light whose circular polarization is in the same sense as that of the incident wave, and

$$dA = 0.8431 \times 10^{-11} \text{ cm.}^2 \sin^4 \frac{\theta}{2} C(\nu) d\Omega \qquad (1.2)$$

for scattered light whose circular polarization is in the opposite sense of the circular polarization of the incident wave. In (1.1) and (1.2) θ is the angle which a vector drawn from the atom, which is supposed to be at the origin of coordinates, to the point of observation makes with the positive z-axis (i.e. θ is the usual polar angle). The function $C(\nu)$ is the shape function for scattering and is given by

$$C(\nu) = \frac{\gamma^2}{(\nu - \nu_1 - \delta)^2 + \gamma^2} \qquad (1.3)$$

where $\nu_1 = 2.4660 \times 10^{15}$ cycles/sec. = frequency of the Lyman-α

line, γ = 252 Mc/sec., and δ = -4281 Mc/sec. The number γ is thus the half-breadth of the scattered line in frequency terms and in wave length terms is 1.03×10^{-4} A. The quantity δ represents a shift in the position of maximum intensity of the scattered radiation from the frequency derived by the Bohr rule from the energy difference of the hydrogen energy levels.

The quantity δ is very interesting, since it contains a large part of the Lamb shift of the ground state. One can, if one wishes, regard the shifting of the frequency of resonance as due to an increase in the energy of the ground state because of the interaction of the atom with the electromagnetic radiation. From the Lamb shift as given in reference 4, the ground state would be raised (in frequency terms) by 8139 Mc/sec. The $\ell = 1$ states are raised only slightly. Hence the Dirac approximation contains more than 50% of the Lamb shift of the ground state. The interpretation of the resonance shift as a change of position of an energy level is discussed in more detail in reference 3. The numerical results strongly suggest that one might be able to obtain the electromagnetic shifts of energy of the hydrogen atom by perturbing about the Dirac approximation. Perhaps some of the infinities associated with the problem will not appear.

Finally, the total cross section for the scattering of radiation near resonance is

$$\sigma(\nu) = 7.062 \times 10^{-11} \text{ cm.}^2 \, C(\nu), \qquad (1.4)$$

when the incident radiation has a frequency ν, whatever its polarization.

2. GENERALIZED DIRAC RESONANCE SCATTERING THEORY

It will be convenient to give a generalization of the Dirac resonance scattering theory and we shall start with a short review of formal scattering theory. Let us consider the Hamiltonian of a scattering system $H = H_o + V$ where V is the interaction.

We shall assume that H_o has a continuous spectrum and we shall denote any point in the continuous spectrum by E. Generally the continuous spectrum will be degenerate and we shall collectively denote the degeneracy variables by the letter s. We shall associate with the continuous spectrum a real positive weight function $w(E,s)$. The operator H_o will also have a discrete spectrum for which we shall denote each eigenvalue by E_i. The corresponding degeneracy will be denoted by d. The values of d are always denumerable, in contrast to the values of the degeneracy variable s which in general may be chosen to be denumerable or non-denumerable. For the purposes of notation we shall act as though s is denumerable and use sums over s although we give ourselves the freedom to interpret s as a continuous variable at our convenience.

The eigenstates of H_o are required to satisfy the completeness relations

$$\sum_{i,d} |E_i,d\rangle\langle E_i,d| + \sum_s \int dE |E,s\rangle w(E,s) \langle E,s| = I, \qquad (2.1)$$

where I is the identity operator in the space and the integration over E is over the entire continuous spectrum.

The orthogonality relations between the eigenfunctions are

$$\langle E_i,d|E_j,d'\rangle = \delta_{ij}\,\delta_{d,d'}$$

$$\langle E,s|E',s'\rangle = [w(E,s)]^{-1}\delta_{s,s'}\delta(E-E') \tag{2.2}$$

$$\langle E,s|E_i,d\rangle = 0$$

For the purposes of scattering theory one is interested in the eigenstates of H which we shall denote by $|E,s)$ and which satisfies the equation

$$|E,s) = |E,s\rangle + \nu_-(E-H_o)V|E,s), \tag{2.3}$$

where

$$\nu_-(x) = \lim_{\epsilon\to 0}\frac{1}{x+i\epsilon} \tag{2.4}$$

From (2.3) and (2.4) it is readily verified that

$$(E-H_o)|E,s) = V|E,s) \tag{2.5}$$

as is required by an eignestate of H. If V is sufficiently "smooth" one can show

$$\lim_{t\to-\infty}\exp[i\tfrac{H_o}{\hbar}t]\exp[-i\tfrac{H}{\hbar}t]|E,s) = |E,s\rangle, \tag{2.6}$$

$$\lim_{t\to+\infty}\exp[i\tfrac{H_o}{\hbar}t]\exp[-i\tfrac{H}{\hbar}t]|E,s) = |E,s\rangle - 2\pi i\delta(E-H_o)V|E,s)$$

as in the usual scattering theory. The matrix elements of the scattering operator S are

$$\langle E,s|S|E',s'\rangle = \delta(E-E')[\delta_{s,s'}-2\pi i\ T(E,s|E,s')], \qquad (2.7)$$

where

$$T(E,s|E',s') = \langle E,s|V|E',s'\rangle \qquad (2.7a)$$

If we designate the state of the system before scattering by $|\Phi_-\rangle$, then the state after scattering is

$$\sum_{s'}\int dE'\ \langle E,s|S|E',s')w(E',s')\langle E's'|\Phi_-\rangle$$

in the representation given by the kets $|E,s\rangle$.

If we take the state before scattering to correspond to a definite value of energy E_o and "direction" s_o, we have

$$|\Phi\rangle = |E_o,s_o\rangle. \qquad (2.8)$$

Then the relative probability per unit time that the particle will be scattered into an interval Δ of the "directions" s from the initial "direction" s_o is

$$\sum_{s \text{ in } \Delta} \frac{2\pi}{\hbar}|T(E_o,s|E_o,s_o)|^2\ w(E_o,s). \qquad (2.9)$$

The expression (2.9) is used to find cross sections if s represents the direction of momentum. One need only divide (2.9) by the flux of particles corresponding to the eigenstate $|E_o,s_o\rangle$.

The usual way to evaluate $T(E,s|E,s')$, which plays the essential role in the scattering phenomena, is to assume V is small and to evaluate (2.3) by iteration. One obtains in this way a series for $|E,s)$ and, from (2.7a) also for $T(E,s|E,s')$. The series is called a "Born expansion" by physicists and a "Neumann expansion" by mathematicians.

However, if any of the point eigenvalues E_i is embedded in the continuous spectrum each term beyond the first of the Born series for $T(E_i,s|E_i,s')$ diverges. The case of resonance scattering of a photon by an atom is precisely a case in which a point eignevalue is embedded in the continuous spectrum and in the case of resonance scattering we are interested in just those values of E near or at E_i.

For the scattering of Lyman-α by hydrogen, the point eigenvalue is the energy of the first excited state of the hydrogen atom. The degeneracy variable d is used to label the angular momentum of the corresponding eigenstate. The part of the continuous spectrum in which we are interested corresponds to having the hydrogen atom in the ground state and to having a photon whose energy is at or near the difference of energies of the first excited state by hydrogen and the ground state. The degeneracy variable s can be selected to specify the direction of the photon together with its circular polarization or s can specify the angular momentum of the photon together with its circular polarization.

Since we have been able to relate photons in an angular momentum basis to those given in the linear momentum basis (reference 5) and give the electromagnetic vector potential in both the linear and angular momentum bases (references 6 and 7), we are able to handle photon wave functions with as much ease as the wave function of any other particle. It seems to us that the previous lack of consistent, simple quantum theory of photons has held up the treatment of resonance scattering of photons which we consider in this paper.

Let us now assume that the point eigenvalue E_1 is embedded in the continuum and that we are interested in resonance scattering at or near E_1. We shall then have to compute $T(E,s|E,s')$ for values of E near or at E_1. In the Dirac approximation, instead of assuming that the entire scattering potential V is small, we assume that all matrix elements of V are small except $\langle E_1,d|V|E,s\rangle$ and $\langle E,s|V|E_1,d\rangle$ for all d and s. In effect the potential V is written

$$V = V_1 + V_2 \tag{2.10}$$

where

$$\langle E_1,d|V_1|E,s\rangle = \langle E,s|V_1|E_1,d\rangle^* = \langle E_1,d|V|E,s\rangle \tag{2.11}$$

where all other matrix elements of V_1 are zero. The interaction V_2 is defined by (2.10) as the difference between V and V_1. It is a remarkable fact that the eigenstates $|E,s)$ obtained when V is replaced by V_1 can be found exactly. Since V_1 is Hermitian,

the scattering operator obtained through its use is unitary. In the Dirac resonance theory we have thus replaced our original problem by an approximate one which can be solved exactly. One can treat V_2 as being small and obtain the eigenstates of H by perturbing about those for $H_o + V_1$.

We shall now obtain the eigenstates $|E,s)$ for $H_o + V_1$ exactly. Our treatment follows that of Dirac closely. Our generalization consists of taking into account the degeneracy of the spectrum.

Accordingly we shall replace V by V_1 in (2.3) and (2.5). Further we shall write

$$\langle E,s|V_1|E_1,d\rangle = \langle E,s|V|E_1 d\rangle = f(E;s,d). \tag{2.12}$$

Then from (2.4), (2.5), (2.1) and the fact that most of the matrix elements of V_1 are zero we obtain

$$\langle E',s'|E,s) = \delta(E-E')\delta_{s,s'}[w(E,s)]^{-1} + \sum_d \gamma_-(E-E')f(E';s',d)\langle E_1,d|E,s), \tag{2.13}$$

and

$$(E-E_1)\langle E_1,d|E,s) = \sum_{s'} \int dE' w(E',s') f^*(E';s',d)\langle E',s'|E,s). \tag{2.14}$$

Equations (2.13) and (2.14) are simultaneous equations for the transformation functions $\langle E_1,d|E,s)$ and $\langle E's'|E,s)$, these two functions giving $|E,s)$ completely in the H_o representation.

On substituting (2.13) into (2.14) we obtain

$$(E-E_1)\langle E_1,d|E,s) = f^*(E;s,d) + \sum_{d's'} \gamma \int dE' w(E',s') f^*(E';s',d) \times$$

$$\gamma_-(E-E')f(E';s',d')\langle E_1,d'|E,s) \tag{2.15}$$

Equation (2.15) is really a set of equations for the functions $\langle E_i, d|E,s)$. It is easy to show that this set of equations has a solution.

We note that

$$\gamma_-(x) = -i\pi\delta(x) + \frac{P}{x} , \tag{2.16}$$

where P means that the principal part is to be used in integrals.

Then we may write

$$\sum_{s'} \int dE'\ w(E',s') f^*(E';s',d)\gamma_-(E-E') f(E';s',d') =$$

$$A_E(d,d') - i\pi\ B_E(d,d') \tag{2.17}$$

where

$$A_E(d,d') = \sum_{s'} \int dE'\ w(E',s')\ \frac{f^*(E';s',d)f(E';s',d')}{E-E'}$$

$$B_E(d,d') = \sum_{s'}\ w(E,s')f^*(E;s',d)f(E;s',d') \tag{2.18}$$

In the integral for $A_E(d,d')$ the principal part is to be taken.

The quantities $A_E(d,d')$ and $B_E(d,d')$ may be regarded as being matrix elements of matrices A_E and B_E respectively, where B_E is a is a positive definite matrix and A_E and B_E are both Hermitian.

There thus exists a non-singular matrix S_E (The subscript shows that this matrix may depend on the energy) such that

$$S_E^{\dagger} A_E S_E = A_{ED}$$

$$S_E^{\dagger} B_E S_E = B_{ED} \tag{2.19}$$

where A_{ED} and R_{ED} are diagonal matrices and the dagger means Hermitian adjoint. Then

$$A_{ED}(d,d') = a(E,d)\delta_{d,d'}$$

$$B_{ED}(d,d') = b(E,d)\delta_{d,d'}. \tag{2.20}$$

In (2.15) let us drop for the moment the variable d and define f(E;s) as being a column vector with components f(E;s,d). Similarly define $\langle E_l | E,s)$ as being a column vector with components $\langle F_l, d | E,s)$.

Then equation (2.15) can be written

$$(E-E_l-A_{ED} + i\pi B_{ED}) S_E^{-1} \langle E_l | E,s) = S_E^{\dagger} f^*(E;s) \tag{2.21}$$

It is now an easy matter to solve for $S_E^{-1} \langle E_l | E,s)$ and hence $\langle E_l | E,s)$. On substituting $\langle E_l | E,s)$ or equivalently $\langle E_l, d | E,s)$ into (2.13), one can solve for $\langle E',s' | E,s)$ and also the scattering operator from (2.7) and (2.7a).

In our problem, the scattering of a photon by a hydrogen atom, H_o is the sum of the Hamiltonian of the hydrogen atom and the

Hamiltonian of the photon field. We take the usual non-relativistic interaction between the photon field and the atom, namely

$$V = - \frac{e}{mc} \underset{\sim}{p} \cdot \underset{\sim}{A} + \frac{e^2}{2mc^2} \underset{\sim}{A}^2$$

where $\underset{\sim}{p}$ is the momentum operator of the electron and $\underset{\sim}{A}$ is the vector potential as given in the radiation gauge.

The matrices corresponding to A_E and B_E in the above treatment are already diagonal if we work in an angular momentum basis for the photon. We anticipate this result because the total angular momentum is a constant of the motion if we ignore recoil of the hydrogen atom as we do (and as is commonly done for emission and absorption of photons by atoms and nuclei unless the radiation is very hard). Then $|E_1,d\rangle$ is a state corresponding to the vacuum for the photon and to having the hydrogen atom in the first excited state. The variable d is chosen to specify the angular momentum quantum number j and the magnetic quantum number m.

The continuous spectrum vector $|E,s\rangle$ corresponds to having the atom in the ground state and to having a single photon whose energy has a value near the energy difference between the first excited state and the ground state. The label d is taken to give the angular quantum number j of the photon, the magnetic quantum number m and the circular polarization of the photon.

Because we are dealing with a single photon, the quadratic term in the vector potential contributes nothing. In reference 7 we have developed the theory of quantization of the photon in terms of an angular momentum basis which parallels closely the technique

of Blatt and Weisskopf (reference 8) for classical electromagnetic radiation. The matrix elements of V_1 simplify considerably because the selection rules are built into the angular momentum representation as in semi-classical treatments. Since the matrices A_E and B_E are diagonal, it is a comparatively simple matter to obtain the scattering operator in the angular momentum representation. The principal difficulty is in evaluating the integral for B_E. We have evaluated this integral exactly without ignoring retardation, as is commonly done in semi-classical treatments of absorption and emission. Indeed the integral diverges if retardation is not taken into account.

We now transform our scattering operator to a linear momentum basis using the results of reference 5. We then assume that the incident wave has a specific momentum and calculate the cross-section using (2.9). Since one has to divide the expression (2.9) by current density of photons a side calculation of the Poynting vector has to be made, which has been done using the results of reference 6.

In the exact calculation γ and δ of equation (1.3) are actually functions of a_o/λ where a_o is the Bohr orbit and λ is the wave length of the light. Since this ratio is very small, the numerical values which we have given represent the leading terms obtained from the exact expression. In a certain sense the calculation of γ and δ is a sort of eigenvalue problem just as the calculation of the energy levels of hydrogen.

In terms of atomic constants we find

$$\sigma(\nu) = \frac{3}{2\pi} \lambda_1^2 C(\nu)$$

and

$$\gamma = 2\left(\frac{2}{3}\right)^5 \alpha^3 \nu_1$$

$$\delta = -\frac{1}{2\pi} \cdot \frac{5}{24} \left(\frac{2}{3}\right)^7 \frac{c}{a_o} \alpha^3$$

where λ_1 is the wave length of Lyman-α radiation = 1.215×10^{-5} cm. $\nu_1 = c/\lambda_1$ = frequency of the Lyman-α radiation, a_o is the radius of the first Bohr orbit, and α is the fine structure constant.

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13. ABSTRACT

The problem of the scattering of a photon by hydrogen in the ground state, when the photon has its principal frequencies near that of Lyman-α radiation, is considered. The scattering operator and cross section for this process are obtained. Dirac's theory of resonance scattering is adapted to the problem and, by quantizing the electromagnetic field in an angular momentum basis, the problem is solved exactly within the framework of the theory. The total scattering cross section at resonance is 7.062×10^{-12} cm^2. The natural half width of the scattered line is 1.03×10^{-4} A. The resonance frequency itself is shifted toward the long wavelength side by 4281 Mcps. The shift in the resonance from the original Lyman-α frequency can be interpreted as an indication that the Dirac resonance scattering theory contains a large part of the Lamb shift of the ground state. This fact suggests new ways of obtaining the Lamb shift for various levels which will be explored in later papers.

14. KEY WORDS

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